

Asymptotic and numerical studies of resonant tunneling in 2D quantum waveguides of variable cross-section

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Abstract

A waveguide coincides with a strip having two narrows of diameter ε . Electron motion is described by the Helmholtz equation with Dirichlet boundary condition. The part of waveguide between the narrows plays the role of resonator and there can occur electron resonant tunneling. This phenomenon consists in the fact that, for an electron with energy E , the probability $T(E)$ to pass from one part of the waveguide to the other part through the resonator has a sharp peak at $E = E_{res}$, where E_{res} denotes a "resonant" energy. In the present paper, we compare the asymptotics of $E_{res} = E_{res}(\varepsilon)$ and $T(E) = T(E, \varepsilon)$ as $\varepsilon \rightarrow 0$ with the corresponding numerical results obtained by approximate computing the waveguide scattering matrix. We show that there exists a band of ε where the asymptotics and numerical results are in close agreement. The numerical calculations become inefficient as ε decreases; however, at such a condition the asymptotics remains reliable. On the other hand, the asymptotics gives way to the numerical method as ε increases; in fact, for wide narrows the resonant tunneling vanishes by itself.

Though, in the present paper, we consider only a 2D waveguide, the applicability of the methods goes far beyond the above simplest model. In particular, the same approach will work for asymptotic and numerical analysis of resonant tunneling in 3D quantum waveguides.

1 Introduction

As an electron propagates in a quantum waveguide of variable cross-section, the waveguide narrows play the role of effective potential barriers for the longitudinal motion. The part of the waveguide between two narrows becomes a "resonator", and there can arise resonant tunneling. It consists of the fact that, for an electron with energy E , the probability $T(E)$ to pass from one part of the waveguide to the other through the resonator has a sharp peak at $E = E_{res}$, where E_{res} denotes a resonant energy. There are prospects for building a new class of nanosize electronics elements (transistors, electron energy monochromators, key devices) based on the phenomenon of resonant tunneling. To analyze their operation, it is important to know E_{res} , the height of the resonant peak, the behavior of $T(E)$ for E close to E_{res} , etc.

In [1], electron propagation was considered in a 3D waveguide with two cylindrical outlets to infinity and two narrows of small diameter ε_1 and ε_2 . The electron motion was described by the Helmholtz equation with Dirichlet boundary condition, radiation condition, and a wave number k between the first and the second thresholds. For the aforementioned characteristics of resonant tunneling, there were obtained asymptotics as $\varepsilon_1, \varepsilon_2 \rightarrow 0$. The

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asymptotic formulas provide mainly a qualitative picture. In the present paper, we show that, being supplemented by some computations, the asymptotics can tell a useful quantitative information as well. Though the paper continues the studies in [1], nevertheless it is practically self-contained; let us explain its goal in detail.

The asymptotic formulas in [1] include several unknown constant coefficients, which can be found by solving some boundary value problems independent of ε_1 and ε_2 . Here, in a model situation, we calculate approximately such coefficients, which enables us to take the asymptotics as numerical values of resonant tunneling characteristics for sufficiently small ε_1 and ε_2 . This leads to the question which ε_1 , ε_2 could be considered as "sufficiently small"; in other words, where does the asymptotics work in a proper way? Though there is no universal answer for such a question, some examples give a grasp of what should be expected in analogous cases. To this end we calculate (also approximately) the scattering matrix and then compare the results obtained by the asymptotic and computational methods independently of one another. Generally, it can be predicted that numerical calculations will become inefficient as the narrow diameters decrease and the resonant peak turns out to be "too sharp"; however, at such a condition the asymptotics should become more reliable. On the other hand, the asymptotics will give way to the numerical method as the narrow diameters increase; in fact, for wide narrows the resonant tunneling would vanish by itself. We observe these phenomena and show that there exists a band of the diameters, where the asymptotic and numerical approaches give compatible results.

In the present paper, we consider a 2D waveguide that is a strip with two narrows of the same diameter ε (see Fig. 2). For 2D waveguides, the asymptotics of resonant tunneling characteristics (as $\varepsilon \rightarrow 0$) are published here for the first time; however, we do not prove the formulas in the paper. The reader could obtain the needed proofs by modifying arguments in [1] related to a 3D situation. Nonetheless, we analyze the structure of asymptotics in order to explain what constants in the asymptotic formulas have to be calculated numerically and how to do that by solving some boundary value problems independent of ε .

The paper consists of five sections. The mathematical model of the waveguide and statement of the problem are given in section 2. The asymptotic formulas are presented in section 3. Then, in section 4, we list the constants to be calculated in the asymptotics, describe the boundary value problems needed for the purpose, and present the methods for solving the problems numerically. In the same section we also describe a method we have used for approximate computation of the waveguide scattering matrix. Finally, section 5 is devoted to comparing basic resonant tunneling characteristics obtained in two different ways, asymptotic and numerical, independent of one another.

Though in the present paper we considered only a 2D waveguide, the applicability of the methods goes far beyond the above simplest model. In particular, the same approach will work for comparison asymptotic and numerical analysis of resonant tunneling in 3D quantum waveguides.

2 Statement of the problem

To describe the domain $G(\varepsilon)$ in \mathbb{R}^2 occupied by the waveguide, we first introduce two auxiliary domains G and Ω in \mathbb{R}^2 . The domain G is the strip

$$G = \mathbb{R} \times D = \{(x, y) \in \mathbb{R}^2 : x \in \mathbb{R} = (-\infty, +\infty); y \in D = (-l/2, l/2)\}.$$

Let us define Ω . Denote by K a double cone with vertex at the origin O that contains the x -axis and is symmetric about the coordinate axes. The set $K \cap S^1$, where S^1 is a unit circle, consists of two simple arcs. Assume that Ω contains the cone K and a neighborhood of its vertex; moreover, outside a large disk (centered at the origin) Ω coincides with K . The boundary $\partial\Omega$ of Ω is supposed to be smooth (see Fig. 1).

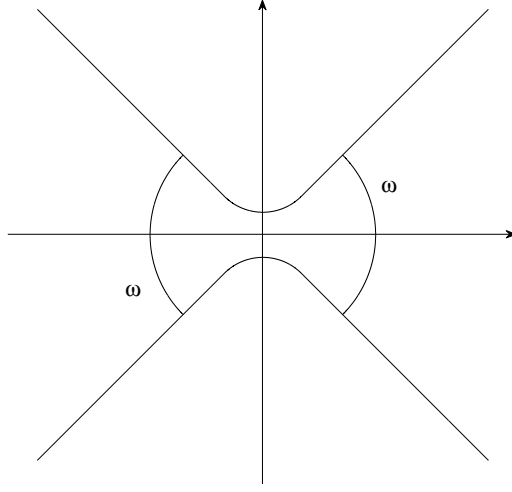


Figure 1: The set Ω .

We now turn to the waveguide $G(\varepsilon)$. Denote by $\Omega(\varepsilon)$ the domain obtained from Ω by the contraction with center at O and coefficient ε . In other words, $(x, y) \in \Omega(\varepsilon)$ if and only if $(x/\varepsilon, y/\varepsilon) \in \Omega$. Let K_j and $\Omega_j(\varepsilon)$ stand for K and $\Omega(\varepsilon)$ shifted by the vector $\mathbf{r}_j = (x_j^0, 0)$, $j = 1, 2$. We assume that $|x_1^0 - x_2^0|$ is sufficiently large so the distance from $\partial K_1 \cap \partial K_2$ to G is positive. We put

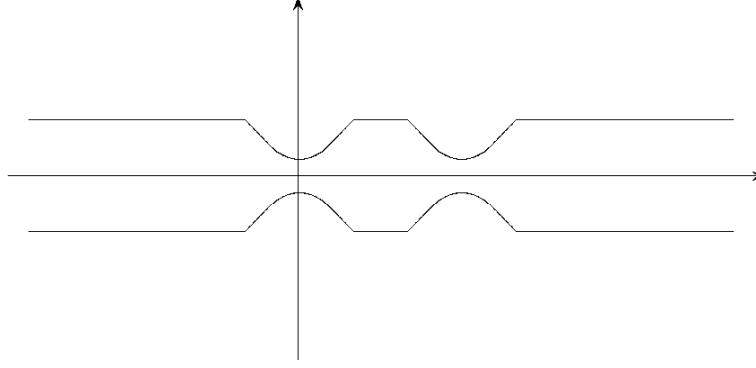
$$G(\varepsilon) = G \cap \Omega_1(\varepsilon) \cap \Omega_2(\varepsilon)$$

(see Fig. 2). The wave function of a free electron of energy k^2 satisfies the boundary value problem

$$\begin{aligned} \Delta u(x, y) + k^2 u(x, y) &= 0, & (x, y) \in G(\varepsilon), \\ u(x, y) &= 0, & (x, y) \in \partial G(\varepsilon). \end{aligned} \quad (2.1)$$

Moreover, u is subject to radiation conditions at infinity. To formulate the conditions we need the problem

$$\begin{aligned} \Delta v(y) + \lambda^2 v(y) &= 0, & y \in D, \\ v(-l/2) = v(l/2) &= 0. \end{aligned} \quad (2.2)$$

Figure 2: The waveguide $G(\varepsilon)$.

The eigenvalues λ_q^2 of this problem, where $q = 1, 2, \dots$ are called the thresholds; they form the sequence $\lambda_q^2 = (\pi q/l)^2$, $q = 1, 2, \dots$. We suppose that k^2 in (2.1) is not a threshold. Given a real k , there exist finitely many linearly independent bounded wave functions. In the linear space spanned by such functions, a basis is formed by the wave functions subject to the radiation conditions

$$\begin{aligned}
 u_m(x, y) &= \begin{cases} e^{i\nu_m x} \Psi_m(y) + \sum_{j=1}^M s_{mj}(k) e^{-i\nu_j x} \Psi_j(y) + O(e^{\delta x}), & x \rightarrow -\infty, \\ \sum_{j=1}^M s_{m,M+j}(k) e^{i\nu_j x} \Psi_j(y) + O(e^{-\delta x}), & x \rightarrow +\infty; \end{cases} \\
 u_{M+m}(x, y) &= \begin{cases} \sum_{j=1}^M s_{M+m,j}(k) e^{-i\nu_j x} \Psi_j(y) + O(e^{\delta x}), & x \rightarrow -\infty, \\ e^{-i\nu_m x} \Psi_m(y) + \sum_{j=1}^M s_{M+m,M+j}(k) e^{i\nu_j x} \Psi_j(y) + O(e^{-\delta x}), & x \rightarrow +\infty. \end{cases}
 \end{aligned} \tag{2.3}$$

Here M is the number of the thresholds satisfying $\lambda^2 < k^2$; $m = 1, 2, \dots, M$; $\nu_m = \sqrt{k^2 - \lambda_m^2}$; Ψ_m is an eigenfunction of the problem (2.2) that corresponds to the eigenvalue λ_m^2 and is chosen so that

$$\Psi_m(y) = \begin{cases} \sqrt{2/l\nu_m} \sin \lambda_m y, & m \text{ even}, \\ \sqrt{2/l\nu_m} \cos \lambda_m y, & m \text{ odd}. \end{cases} \tag{2.4}$$

The function $U_j(x, y) = e^{i\nu_j x} \Psi_j(y)$, $j = 1, \dots, M$, in the strip G is a wave incoming from $-\infty$ and outgoing to $+\infty$, while $U_{M+j}(x, y) = e^{-i\nu_j x} \Psi_j(y)$, $j = 1, \dots, M$, is a wave going from $+\infty$ to $-\infty$. The scattering matrix

$$S = \|s_{mj}\|_{m,j=1,\dots,2M}$$

is unitary. The values

$$R_m = \sum_{j=1}^M |s_{mj}|^2, \quad T_m = \sum_{j=1}^M |s_{m,M+j}|^2$$

are called the reflection and transition coefficients, relatively, for the wave U_m incoming to $G(\varepsilon)$ from $-\infty$, $m = 1, \dots, M$. (Similar definitions can be given for the wave U_{M+m} coming from $+\infty$.)

In the present work we will discuss only the case $(\pi/l)^2 < k^2 < (2\pi/l)^2$, i.e., k^2 is between the first and the second thresholds. Then the scattering matrix is of size 2×2 . We consider only the scattering of the wave incoming from $-\infty$ and denote the reflection and transition coefficients as

$$R = R(k, \varepsilon) = |s_{11}(k, \varepsilon)|^2, \quad T = T(k, \varepsilon) = |s_{12}(k, \varepsilon)|^2. \quad (2.5)$$

The goal is to find a "resonant" value $k_r = k_r(\varepsilon)$ of the parameter k corresponding to the maximum of the transition coefficient, and to describe the behavior of $T(k, \varepsilon)$ for k in a neighborhood of $k_r(\varepsilon)$ as $\varepsilon \rightarrow 0$.

3 Outline of the asymptotics

When deriving an asymptotics of a wave function (i.e. solution of problem (2.1)) as $\varepsilon \rightarrow 0$, we use the compound asymptotics method (the general theory of the method was exposed, e.g., in [2], [3]). To this end we introduce "limit" boundary value problems independent of the parameter ε . Put $G(0) = G \cap K_1 \cap K_2$ (Fig. 3); thus, $G(0)$ consists of the three parts G_1 , G_2 , and G_3 , where G_1 and G_3 are infinite domains while G_2 is a bounded resonator.

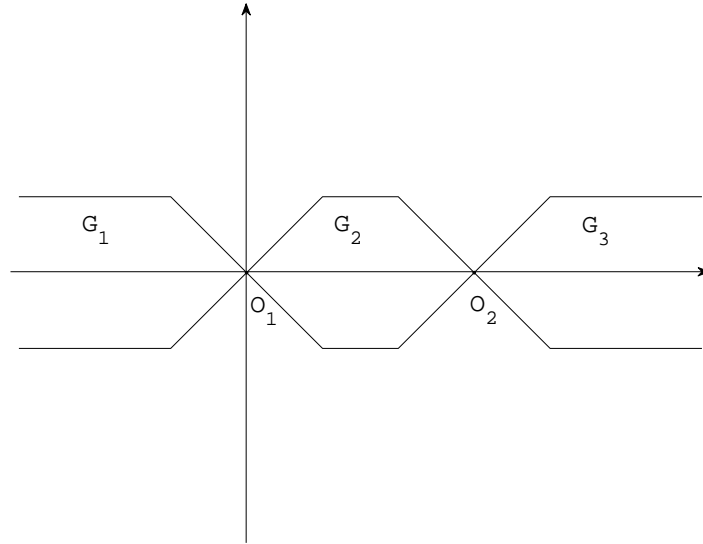


Figure 3: The set $G(0)$.

The problems

$$\begin{aligned} \Delta v(x, y) + k^2 v(x, y) &= 0, & (x, y) \in G_j, \\ v(x, y) &= 0, & (x, y) \in \partial G_j, \end{aligned} \quad (3.1)$$

where $j = 1, 2, 3$ and ∂G_j is the boundary of G_j , are called the first kind limit problems. Solutions v_1 and v_3 are subject to some radiation conditions at infinity and all three functions v_1, v_2, v_3 satisfy some conditions at the corner points. All of the conditions will be formulated as required.

Let us turn to the domains Ω_1 and Ω_2 (see Fig. 1). Problems of the form

$$\begin{aligned} \Delta w(\xi_j, \eta_j) &= F(\xi_j, \eta_j) & \text{in } \Omega_j, \\ w(\xi_j, \eta_j) &= 0 & \text{on } \partial\Omega_j, \end{aligned} \quad (3.2)$$

are called the second kind limit problems. We seek solutions of the problems satisfying

$$w(\xi_j, \eta_j) = O\left(\rho_j^{-3\pi/\omega_j}\right) \quad \text{as } \rho_j \rightarrow \infty;$$

here (ξ_j, η_j) are rectangular coordinates with origin at the vertex O_j of K_j , ρ_j being the distance from (ξ_j, η_j) to O_j and ω_j the opening of K_j , $j = 1, 2$.

In the waveguide $G(\varepsilon)$, we consider the scattering of the wave $U(x, y) = e^{i\nu_1 x} \Psi_1(y)$ incoming from $-\infty$ (see (2.4)). The asymptotics of the wave function is the main technical result. Although rather cumbersome, it will lead to much more explicit characteristics of the process. The wave function admits the representation

$$\begin{aligned} u(x, y; \varepsilon) &= \chi_{1,\varepsilon}(x, y)v_1(x, y; \varepsilon) + \\ &+ \Theta(r_1)w_1(\varepsilon^{-1}x_1, \varepsilon^{-1}y_1; \varepsilon) + \chi_{2,\varepsilon}(x, y)v_2(x, y; \varepsilon) + \\ &+ \Theta(r_2)w_2(\varepsilon^{-1}x_2, \varepsilon^{-1}y_2; \varepsilon) + \chi_{3,\varepsilon}(x, y)v_3(x, y; \varepsilon) + R(x, y; \varepsilon). \end{aligned} \quad (3.3)$$

Let us explain the notation and the structure of this formula. When composing the formula, we first describe the behavior of the wave function to the right of the narrows, where the wave function can be approximated by a solution v_3 of the problem (3.1) in G_3 . The solution is subject to the radiation condition

$$v_3(x, y; \varepsilon) \sim s_{12}(\varepsilon)e^{i\nu_1 x} \Psi_1(y) \quad \text{as } x \rightarrow +\infty, \quad (3.4)$$

the element $s_{12}(\varepsilon)$ of scattering matrix being yet unknown. Problem (3.1) does not contain ε , nevertheless v_3 depends on the parameter because of $s_{12}(\varepsilon)$. By $\chi_{3,\varepsilon}$ we denote a cut-off function defined by

$$\chi_{3,\varepsilon}(x, y) = (1 - \Theta(r_2/\varepsilon)) \mathbf{1}_{G_3}(x, y),$$

where $r_2 = \sqrt{x_2^2 + y_2^2}$ and (x_2, y_2) are the coordinates of a point (x, y) in the system obtained by shifting the origin to the point O_2 ; $\mathbf{1}_{G_3}$ is the indicator of G_3 (equal to 1 in G_3 and to 0 outside G_3); $\Theta(\rho)$ is a smooth non-negative function on the half-axis $0 \leq \rho < +\infty$ that equals 1 as $0 \leq \rho \leq \delta$ and vanishes as $\rho \geq 2\delta$ (δ being a fixed small positive number). Thus $\chi_{3,\varepsilon}$ is defined on the whole waveguide $G(\varepsilon)$ as well as the function $\chi_{3,\varepsilon}v_3$ in (3.3).

Being substituted to (2.1), the function $\chi_{3,\varepsilon}v_3$ gives a discrepancy in the right-hand side of the Helmholtz equation; the discrepancy is supported near the second narrow (to the right of it). We compensate the principal part of the discrepancy by means of the second kind limit problem in the domain Ω_2 . Namely, the discrepancy is rewritten into coordinates (ξ_2, η_2) in Ω_2 and is taken as a right-hand side for the Laplace equation. The solution w_2 of

the corresponding problem (3.2) has to be rewritten into coordinates (x_2, y_2) and multiplied by a cut-off function. As a result, there arises the term $\Theta(r_2)w_2(\varepsilon^{-1}x_2, \varepsilon^{-1}y_2; \varepsilon)$ in (3.3).

Now we substitute the sum of two obtained terms into (2.1). The principal part of the corresponding discrepancy is supported in G_2 near the second narrow. We compensate it by solving the problem (3.1) in G_2 and obtain the term $\chi_{2,\varepsilon}(x, y)v_2(x, y; \varepsilon)$ with

$$\chi_{2,\varepsilon}(x, y) = (1 - \Theta(\varepsilon^{-1}r_1) - \Theta(\varepsilon^{-1}r_2)) \mathbf{1}_{G_2}(x, y).$$

Then in a similar way there arise

$$\Theta(r_1)w_1(\varepsilon^{-1}x_1, \varepsilon^{-1}y_1; \varepsilon) \text{ and } \chi_{1,\varepsilon_1}(x, y)v_1(x, y; \varepsilon).$$

At the last step, we find the function v_1 that satisfies both the limit problem (3.1) in G_1 and the radiation condition

$$v_1(x, y; \varepsilon) \sim s_{12}(\varepsilon)\alpha(\varepsilon)e^{i\nu_1x}\Psi_1(y) + s_{12}(\varepsilon)\beta(\varepsilon)e^{-i\nu_1x}\Psi_1(y)$$

as $x \rightarrow -\infty$. The coefficients α, β and the entries s_{11}, s_{12} of the scattering matrix turn out to be uniquely determined by a relation between α and β that assures compensation of the principal part of the discrepancy arising in the problem in G_1 , and by requirements

$$s_{12}(\varepsilon)\alpha(\varepsilon) = 1, \quad s_{12}(\varepsilon)\beta(\varepsilon) = s_{11}(\varepsilon).$$

The remainder $R(x, y; \varepsilon)$ is small in comparison with the principal part of (3.3) as $\varepsilon \rightarrow 0$.

We specify (3.3) provided k^2 varies in an interval containing a unique simple eigenvalue k_0^2 of the problem (3.1) in G_2 .

1. Introduce a special solution \mathbf{v}_3 of the problem (3.1) in G_3 satisfying

$$\mathbf{v}_3(x, y) \sim (r_2^{-\pi/\omega} + ar_2^{\pi/\omega})\Phi(\varphi_2) \quad \text{as } r_2 \rightarrow 0$$

(here and below, (r_j, φ_j) are polar coordinates with center at O_j , $j = 1, 2$; $\Phi(\varphi) = \cos(\pi\varphi/\omega)$), and

$$\mathbf{v}_3(x, y) \sim Ae^{i\nu_1x}\Psi_1(y) \quad \text{as } x \rightarrow +\infty.$$

These conditions define \mathbf{v}_3 uniquely. The constants a, A (depending on k and on the geometry of G_3) have to be calculated. We have

$$v_3(x, y; \varepsilon) = \frac{s_{12}(\varepsilon)}{A}\mathbf{v}_3(x, y).$$

2. Consider a solution w_r of the homogeneous problem (3.2) satisfying

$$w_r(\xi, \eta) = \begin{cases} (\rho^{\pi/\omega} + \alpha\rho^{-\pi/\omega})\Phi(\varphi) + O(\rho^{-3\pi/\omega}), & \text{as } \rho \rightarrow \infty, \xi > 0; \\ \beta\rho^{-\pi/\omega}\Phi(\pi - \varphi) + O(\rho^{-3\pi/\omega}), & \text{as } \rho \rightarrow \infty, \xi < 0. \end{cases} \quad (3.5)$$

The constants α, β (depending on Ω) have to be calculated. One can prove that $\beta \neq 0$ (cf. [1], proof of Proposition 3.4). We put

$$\mathbf{w}^-(\xi, \eta) = \frac{1}{\beta} (w_r(\xi, \eta) - \zeta_r(\xi, \eta)(\rho^{\pi/\omega} + \alpha\rho^{-\pi/\omega})\Phi(\varphi) - \zeta_l(\xi, \eta)\beta\rho^{-\pi/\omega}\Phi(\pi - \varphi)),$$

where ζ_r is a cut-off function equal to 1 as $\xi > 0$ and 0 as $\xi < 0$, $\zeta_l(\xi, \eta) = \zeta_r(-\xi, \eta)$. We also put

$$\mathbf{w}^+(\xi, \eta) = \beta \mathbf{w}^-(\xi, \eta) - \alpha \mathbf{w}^-(\xi, \eta).$$

Then

$$w_2(\xi_2, \eta_2; \varepsilon) = \frac{s_{12}(\varepsilon)}{A} (\varepsilon^{-\pi/\omega} \mathbf{w}^-(\xi_2, \eta_2) + a \varepsilon^{\pi/\omega} \mathbf{w}^+(\xi_2, \eta_2)).$$

3. Remind that k_0^2 is a simple eigenvalue. Let v_0 be an eigenfunction corresponding to k_0^2 and normalized by $\int_{G_2} |v_0|^2 dx dy = 1$. We have

$$v_0(x, y) \sim \begin{cases} b_1 r_1^{\pi/\omega} \Phi(\varphi_1), & \text{as } r_1 \rightarrow 0; \\ b_2 r_2^{\pi/\omega} \Phi(\pi - \varphi_2), & \text{as } r_2 \rightarrow 0. \end{cases} \quad (3.6)$$

In what follows we assume that $b_1 \neq 0$; such an assumption is fulfilled, for example, if k_0^2 is the first eigenvalue of problem (3.1). Since G_2 is invariant with respect to the transformation $(x, y) \mapsto (d - x, y)$, while $d = |x_1^0 - x_2^0|$ is the distance between O_1 and O_2 , one can prove that $q := b_2/b_1 = \pm 1$. Introduce special solutions $\mathbf{v}_{21}, \mathbf{v}_{22}$ of the problem (3.1) in G_2 satisfying

$$\begin{aligned} \mathbf{v}_{21}(x, y) &\sim \begin{cases} ((k^2 - k_0^2) r_1^{-\pi/\omega} + c_1 r_1^{\pi/\omega}) \Phi(\varphi_1), & \text{as } r_1 \rightarrow 0; \\ c_2 r_2^{\pi/\omega} \Phi(\pi - \varphi_2), & \text{as } r_2 \rightarrow 0, \end{cases} \\ \mathbf{v}_{22}(x, y) &\sim \begin{cases} (b_2 r_1^{-\pi/\omega} + d_1 r_1^{\pi/\omega}) \Phi(\varphi_1), & \text{as } r_1 \rightarrow 0; \\ (-b_1 r_2^{-\pi/\omega} + d_2 r_2^{\pi/\omega}) \Phi(\pi - \varphi_2), & \text{as } r_2 \rightarrow 0. \end{cases} \end{aligned}$$

The coefficients c_1, c_2, d_1, d_2 depend on k and on G_2 . One can prove that $c_j(k_0) = b_1 b_j$. Then

$$v_2(x, y; \varepsilon) = \frac{s_{12}(\varepsilon)}{b_1 c_2} ((b_1 \gamma(\varepsilon) - d_2 \delta(\varepsilon)) \mathbf{v}_{21}(x, y) + c_2 \delta(\varepsilon) \mathbf{v}_{22}(x, y)),$$

where

$$\gamma(\varepsilon) = \frac{1}{A\beta} (\varepsilon^{-2\pi/\omega} - a\alpha), \quad \delta(\varepsilon) = -\frac{1}{A\beta} (\alpha + a(\beta^2 - \alpha^2) \varepsilon^{2\pi/\omega}). \quad (3.7)$$

4. We have

$$w_1(\xi_1, \eta_1; \varepsilon) = \frac{1}{|A|^2} ((\bar{A} s_{11}(\varepsilon) + A) \varepsilon^{-\pi/\omega} \mathbf{w}^-(\xi_1, \eta_1) + (a \bar{A} s_{11}(\varepsilon) + \bar{a} A) \varepsilon^{\pi/\omega} \mathbf{w}^+(\xi_1, \eta_1)),$$

where s_{11} is defined by (3.8) below.

5. Introduce a special solution \mathbf{v}_1 of the problem (3.1) in G_1 by $\mathbf{v}_1(x_1, y_1) = \mathbf{v}_3(d - x_1, y_1)$. Then

$$v_1(x, y; \varepsilon) = \frac{s_{11}(\varepsilon)}{A} \mathbf{v}_1(x, y) + \frac{1}{\bar{A}} \bar{\mathbf{v}}_1(x, y),$$

where

$$s_{11}(\varepsilon) = (2ib_1c_2)^{-1}((k^2 - k_0^2)b_1|\gamma(\varepsilon)|^2 - ((k^2 - k_0^2)d_2 - b_2c_2)\overline{\gamma(\varepsilon)}\delta(\varepsilon) + b_1c_1\gamma(\varepsilon)\overline{\delta(\varepsilon)} - (c_1d_2 - c_2d_1)|\delta(\varepsilon)|^2)s_{12}(\varepsilon), \quad (3.8)$$

$$s_{12}(\varepsilon) = 2ib_1c_2(-(k^2 - k_0^2)b_1\gamma(\varepsilon)^2 + ((k^2 - k_0^2)d_2 - b_1c_1 - b_2c_2)\gamma(\varepsilon)\delta(\varepsilon) + (c_1d_2 - c_2d_1)\delta(\varepsilon)^2)^{-1}, \quad (3.9)$$

while $\gamma(\varepsilon)$, $\delta(\varepsilon)$ are defined by (3.7). One can verify that $|s_{11}|^2 + |s_{12}|^2 = 1$ (cf. [1]).

Analysis of (3.9) shows that $T = T(k, \varepsilon) = |s_{12}|^2$ has a sharp peak at $k = k_{res}$,

$$k_{res}^2 = k_0^2 - 2\alpha b_1^2 \varepsilon^{2\pi/\omega} + O(\varepsilon^{2\pi/\omega+\tau}), \quad (3.10)$$

where $\tau = \min\{\pi/\omega, 2 - \sigma\}$, σ being a small positive number. Suppose that k varies in a small neighborhood I of k_{res} , $I = \{k : |k - k_{res}| \leq c\varepsilon^{2\pi/\omega+p}\}$, $p > 0$. Then (3.9) takes the form

$$s_{12}(k, \varepsilon) = \frac{q(A(k_0)/|A(k_0)|)^2}{1 - iP\left(\frac{k^2 - k_{res}^2}{\varepsilon^{4\pi/\omega}}\right)}(1 + O(\varepsilon^p)),$$

where $P = (2b_1^2\beta^2|A(k_0)|^2)^{-1}$. Hence,

$$T(k, \varepsilon) = \frac{1}{1 + P^2\left(\frac{k^2 - k_{res}^2}{\varepsilon^{4\pi/\omega}}\right)^2}(1 + O(\varepsilon^p)). \quad (3.11)$$

The width of the peak at its half-height (the so-called a resonator quality factor) is

$$\Upsilon(\varepsilon) = \frac{2}{P}\varepsilon^{4\pi/\omega}. \quad (3.12)$$

4 Problems and methods for numerical analysis

The principal parts of asymptotic formulas (3.10) – (3.12) for the main characteristics of resonant tunneling contain the constants b_1 , $|A|$, α , β . To find the constants we have to solve numerically several boundary value problems. In this section, we state the problems and describe a way to solve them. We also outline a method for computing the waveguide scattering matrix S .

To find b_1 , we solve the spectral problem (3.1) in G_2 by FEM as usual. Let V_0 be an eigenfunction corresponding to k_0^2 and normalized by $\int_{G_2} |V_0(x, y)|^2 dx dy = 1$. Then b_1 in (3.6) can be defined by

$$b_1 = \varepsilon^{-\pi/\omega} \frac{V_0(\varepsilon, 0)}{\Phi(0)} = \sqrt{\pi} \varepsilon^{-\pi/\omega} V_0(\varepsilon, 0).$$

Let us calculate $|A|$. In order to avoid dealing with \mathbf{v}_1 , which increases at O_1 , we introduce $\mathbf{v} = (\mathbf{v}_1 - \overline{\mathbf{v}}_1)/A$,

$$\mathbf{v}(x_1, y_1) = \begin{cases} \mathbf{a}r_1^{\pi/\omega}\Phi(\varphi_1) & \text{as } r_2 \rightarrow 0; \\ \left(e^{-i\nu_1x_1} + \frac{\overline{A}}{A}e^{i\nu_1x_1}\right)\Psi_1(y_1) + O(e^{-\delta|x_1|}) & \text{as } x_1 \rightarrow -\infty, \end{cases} \quad (4.1)$$

where $\mathbf{a} = 2i\text{Im } a/A$. According to Lemma 4.1 in [1], $\text{Im } a = |A|^2$, so $\mathbf{a} = 2i\bar{A}$. Thus, it suffices to calculate \mathbf{a} . Denote the truncated domain $G_1 \cap \{(x_1, y_1) : x_1 > -R\}$ by G_1^R and the artificial part of the boundary $\partial G_1^R \cap \{(x_1, y_1) : x_1 = -R\}$ by Γ^R . Let V be a solution of the problem

$$\begin{aligned} \Delta V(x_1, y_1) + k^2 V(x_1, y_1) &= 0, & (x_1, y_1) \in G_1^R; \\ V(x_1, y_1) &= 0, & (x_1, y_1) \in \partial G_1^R \setminus \Gamma^R; \\ \partial_n V(x_1, y_1) + i\nu_1 V(x_1, y_1) &= 2i\nu_1 e^{i\nu_1 R} \Psi_1(y_1), & (x_1, y_1) \in \Gamma^R. \end{aligned} \quad (4.2)$$

We find V with FEM and put

$$\mathbf{a} = \sqrt{\pi} \varepsilon^{-\pi/\omega} V(-\varepsilon, 0).$$

Pass to description of a boundary value problem for calculating α, β in (3.5). Denote $\Omega \cap \{(r, \varphi) : r < R\}$ by Ω^R and $\partial\Omega \cap \{(r, \varphi) : r = R\}$ by Γ^R . Consider the problem

$$\begin{aligned} \Delta w(\xi, \eta) &= 0, & (\xi, \eta) \in \Omega^R; \\ w(\xi, \eta) &= 0, & (\xi, \eta) \in \partial\Omega^R \setminus \Gamma^R; \\ \partial_n w(\xi, \eta) + \zeta w(\xi, \eta) &= g(\xi, \eta), & (\xi, \eta) \in \Gamma^R. \end{aligned} \quad (4.3)$$

If w is a solution and $\zeta > 0$, then

$$\|w; L_2(\Gamma^R)\| \leq \zeta^{-1} \|g; L_2(\Gamma^R)\|. \quad (4.4)$$

Indeed, substitute $u = v = w$ to the Green formula

$$\begin{aligned} (\Delta u, v)_{\Omega^R} &= (\partial_n u, v)_{\partial\Omega^R} - (\nabla u, \nabla v)_{\Omega^R} \\ &= (\partial_n u, v)_{\partial\Omega^R \setminus \Gamma^R} + (\partial_n u + \zeta u, v)_{\Gamma^R} - \zeta(u, v)_{\Gamma^R} - (\nabla u, \nabla v)_{\Omega^R} \end{aligned}$$

and get

$$0 = (g, w)_{\Gamma^R} - \zeta \|w; L_2(\Gamma^R)\|^2 - \|\nabla w; L_2(\Omega^R)\|^2.$$

From this and the obvious chain of inequalities

$$\zeta \|w; L_2(\Gamma^R)\|^2 \leq \zeta \|w; L_2(\Gamma^R)\|^2 + \|\nabla w; L_2(\Omega^R)\|^2 = (g, w)_{\Gamma^R} \leq \|w; L_2(\Gamma^R)\| \|g; L_2(\Gamma^R)\|$$

we obtain (4.4). Denote the left part of Γ^R by Γ_-^R and the right part of Γ^R by Γ_+^R . Let W be the solution of (4.3) as $\zeta = \pi/\omega R$, $g|_{\Gamma_-^R} = 0$, $g|_{\Gamma_+^R} = (2\pi/\omega) R^{(\pi/\omega)-1} \Phi(\varphi)$. Since the asymptotics (3.5) can be differentiated, $w_r - W$ satisfies (4.3) with $g = O(R^{-(3\pi/\omega)-1})$. According to (4.4),

$$\|w_r - W; L_2(\Gamma^R)\| \leq c \frac{\omega R}{\pi} R^{-(3\pi/\omega)-1} = c' R^{-3\pi/\omega}$$

as $R \rightarrow +\infty$. We find W with FEM and take

$$\beta = \frac{W(-R, 0)}{\Phi(0)} R^{\pi/\omega} = \sqrt{\pi} W(-R, 0) R^{\pi/\omega}.$$

Obviously, $\|(w_r - R^{\pi/\omega}\Phi(\varphi)) - (W - R^{\pi/\omega}\Phi(\varphi)); L_2(\Gamma^R)\| \leq c'R^{-3\pi/\omega}$, therefore we put

$$\alpha = \frac{W(R, 0) - R^{\pi/\omega}\Phi(0)}{\Phi(0)} R^{\pi/\omega} = \sqrt{\pi}W(R, 0)R^{\pi/\omega} - R^{2\pi/\omega}.$$

Finally, we outline the method of calculating the scattering matrix. Introduce the notation

$$G(\varepsilon, R) = G(\varepsilon) \cap \{(x, y) : -R < x < d + R\}, \\ \Gamma_1^R = \partial G(\varepsilon, R) \cap \{(x, y) : x = -R\}, \quad \Gamma_2^R = \partial G(\varepsilon, R) \cap \{(x, y) : x = d + R\}$$

for large R . We search the row $(s_{m1}, \dots, s_{m,2M})$ of the scattering matrix $s = s(k)$ defined by (2.3), $m = 1, \dots, M$. As approximation to the row we take the minimizer of a quadratic functional. To construct such a functional we consider the problem

$$\begin{aligned} \Delta \mathcal{X}_m^R + k^2 \mathcal{X}_m^R &= 0 \quad \text{in } G(\varepsilon, R), \\ \mathcal{X}_m^R &= 0 \quad \text{on } \partial G(\varepsilon, R) \setminus (\Gamma_1^R \cup \Gamma_2^R), \\ (\partial_n + i\zeta) \mathcal{X}_m^R &= i(-\nu_m + \zeta)e^{-i\nu_m R} \Psi_m(y) + \sum_{j=1}^M a_j i(\nu_j + \zeta)e^{i\nu_j R} \Psi_j(y) \quad \text{on } \Gamma_1^R, \\ (\partial_n + i\zeta) \mathcal{X}_m^R &= \sum_{j=1}^M a_{M+j} i(\nu_j + \zeta)e^{i\nu_j(d+R)} \Psi_j(y) \quad \text{on } \Gamma_2^R, \end{aligned} \quad (4.5)$$

where $\zeta \in \mathbb{R} \setminus \{0\}$ is an arbitrary fixed number, and a_1, \dots, a_M are complex numbers. The solution u_m to the homogeneous problem (2.1) satisfies the first two equations (4.5). The asymptotics (2.3) can be differentiated so u_m satisfies the last two equations in (4.5) up to an exponentially small discrepancy. As approximation for the row $(s_{m1}, \dots, s_{m,2M})$ we take the minimizer $a^0(R) = (a_1^0(R), \dots, a_{2M}^0(R))$ of the functional

$$\begin{aligned} J_m^R(a_1, \dots, a_{2M}) &= \|\mathcal{X}_m^R - e^{-i\nu_m R} \Psi_m - \sum_{j=1}^M a_j e^{i\nu_j R} \Psi_j; L_2(\Gamma_1^R)\|^2 \\ &+ \|\mathcal{X}_m^R - \sum_{j=1}^M a_{M+j} e^{i\nu_j(d+R)} \Psi_j; L_2(\Gamma_2^R)\|^2, \end{aligned} \quad (4.6)$$

where \mathcal{X}_m^R is a solution to problem (4.5). As shown in [4], $a_j^0(R, k) \rightarrow s_{mj}(k)$ with exponential rate as $R \rightarrow \infty$ and $j = 1, \dots, 2M$. To find the dependence of \mathcal{X}_m^R on a_1, \dots, a_{2M} , we consider the problems

$$\begin{aligned} \Delta v_j^\pm + k^2 v_j^\pm &= 0 \quad \text{in } G(\varepsilon, R), \\ v_j^\pm &= 0 \quad \text{on } \partial G(\varepsilon, R) \setminus (\Gamma_1^R \cup \Gamma_2^R), \\ (\partial_n + i\zeta) v_j^\pm &= i(\mp \nu_j + \zeta)e^{\mp i\nu_j R} \Psi_j \quad \text{on } \Gamma_1^R, \\ (\partial_n + i\zeta) v_j^\pm &= 0 \quad \text{on } \Gamma_2^R; \quad j = 1, \dots, M; \end{aligned} \quad (4.7)$$

and

$$\begin{aligned} \Delta v_j^\pm + k^2 v_j^\pm &= 0 \quad \text{in } G(\varepsilon, R), \\ v_j^\pm &= 0 \quad \text{on } \partial G(\varepsilon, R) \setminus (\Gamma_1^R \cup \Gamma_2^R), \\ (\partial_n + i\zeta) v_j^\pm &= 0 \quad \text{on } \Gamma_1^R, \\ (\partial_n + i\zeta) v_j^\pm &= i(\mp \nu_j + \zeta)e^{\mp i\nu_j(d+R)} \Psi_j \quad \text{on } \Gamma_2^R; \quad j = M+1, \dots, 2M. \end{aligned} \quad (4.8)$$

Express \mathcal{X}_m^R by means of the solutions $v_j^\pm = v_{j,R}^\pm$ to problems (4.7)–(4.8). We have $\mathcal{X}_m^R = v_{m,R}^+ + \sum_j a_j v_{j,R}^-$. Let us introduce the $2M \times 2M$ -matrices with entries

$$\begin{aligned}\mathcal{E}_{mj}^R &= ((v_m^- - e^{i\nu_m R} \Psi_m), (v_j^- - e^{i\nu_j R} \Psi_j))_{\Gamma_1^R} + (v_m^-, v_j^-)_{\Gamma_2^R}, \\ \mathcal{E}_{m,M+j}^R &= ((v_m^- - e^{i\nu_m R} \Psi_m), v_{M+j}^-)_{\Gamma_1^R} + (v_m^-, (v_{M+j}^- - e^{i\nu_j(d+R)} \Psi_j))_{\Gamma_2^R}, \\ \mathcal{E}_{M+m,j}^R &= (v_{M+m}^-, (v_j^- - e^{i\nu_j R} \Psi_j))_{\Gamma_1^R} + ((v_{M+m}^- - e^{i\nu_m(d+R)} \Psi_m), v_j^-)_{\Gamma_2^R}, \\ \mathcal{E}_{M+m,M+j}^R &= (v_{M+m}^-, v_{M+j}^-)_{\Gamma_1^R} + ((v_{M+m}^- - e^{i\nu_m(d+R)} \Psi_m), (v_{M+j}^- - e^{i\nu_j(d+R)} \Psi_j))_{\Gamma_2^R}; \\ \mathcal{F}_{mj}^R &= ((v_m^+ - e^{-i\nu_m R} \Psi_m), (v_j^- - e^{i\nu_j R} \Psi_j))_{\Gamma_1^R} + (v_m^+, v_j^-)_{\Gamma_2^R}, \\ \mathcal{F}_{m,M+j}^R &= ((v_m^+ - e^{-i\nu_m R} \Psi_m), v_{M+j}^-)_{\Gamma_1^R} + (v_m^+, (v_{M+j}^- - e^{i\nu_j(d+R)} \Psi_j))_{\Gamma_2^R}, \\ \mathcal{F}_{M+m,j}^R &= (v_{M+m}^+, (v_j^- - e^{i\nu_j R} \Psi_j))_{\Gamma_1^R} + ((v_{M+m}^+ - e^{-i\nu_m(d+R)} \Psi_m), v_j^-)_{\Gamma_2^R}, \\ \mathcal{F}_{M+m,M+j}^R &= (v_{M+m}^+, v_{M+j}^-)_{\Gamma_1^R} + ((v_{M+m}^+ - e^{-i\nu_m(d+R)} \Psi_m), (v_{M+j}^- - e^{i\nu_j(d+R)} \Psi_j))_{\Gamma_2^R},\end{aligned}$$

$j, m = 1, \dots, M$. We also put

$$\begin{aligned}\mathcal{G}_m^R &= ((v_m^+ - e^{-i\nu_m R} \Psi_m), (v_m^+ - e^{-i\nu_j R} \Psi_j))_{\Gamma_1^R} + (v_m^+, v_m^+)_{\Gamma_2^R}, \\ \mathcal{G}_{M+m}^R &= (v_{M+m}^+, v_{M+m}^+)_{\Gamma_1^R} + ((v_{M+m}^+ - e^{-i\nu_m(d+R)} \Psi_m), (v_{M+m}^+ - e^{-i\nu_j(d+R)} \Psi_j))_{\Gamma_2^R},\end{aligned}$$

$m=1, \dots, M$. The functional (4.6) can be written in the form

$$J_m^R(a, k) = \langle a \mathcal{E}^R(k), a \rangle + 2\text{Re} \langle \mathcal{F}_m^R(k), a \rangle + \mathcal{G}_m^R(k),$$

where \mathcal{F}_m^R is the m -th row of the matrix \mathcal{F}^R and $\langle \cdot, \cdot \rangle$ is the inner product on \mathbb{C}^M . The minimizer $a^0 = a^0(R, k)$ (a row) satisfies $a^0 \mathcal{E}^R + \mathcal{F}_m^R = 0$. Recall that we are searching the m -th row of the scattering matrix as $m = 1, \dots, M$. Along the same arguments one can prove that the found minimizer for $m = M+1, \dots, 2M$ serves as approximation to the m -th row of the scattering matrix. Therefore, as approximation $s^R(k)$ for the scattering matrix $s(k)$ we take a solution to the equation $s^R \mathcal{E}^R + \mathcal{F}^R = 0$.

When $M = 1$, i.e. k^2 is between the first and the second thresholds, we take $\zeta = -\nu_1$. Then $v_1^- = v_2^- = 0$, $\mathcal{E}^R = (1/\nu_1)\text{Id}$, and $s^R = -\nu_1 \mathcal{F}^R$.

5 Comparison of asymptotic and numerical results

Let us compare the asymptotics $k_{res,a}^2(\varepsilon)$ of resonant energy $k_{res}^2(\varepsilon)$ and the approximate value $k_{res,n}^2(\varepsilon)$ obtained by numerical method. Fig. 4 shows good agreement with the values for $0.1 \leq \varepsilon \leq 0.5$. We have

$$|k_{res,a}^2(\varepsilon) - k_{res,n}^2(\varepsilon)|/k_{res,a}^2(\varepsilon) \leq 10^{-3}$$

for $0.1 \leq \varepsilon \leq 0.3$ and only for $\varepsilon = 0.5$ the ratio approaches $2 \cdot 10^{-2}$. For $\varepsilon < 0.1$ the numerical method is ill-conditioned.

The difference between the asymptotic and numerical values is more significant for larger ε because the asymptotics becomes not reliable. However, as the numerical method

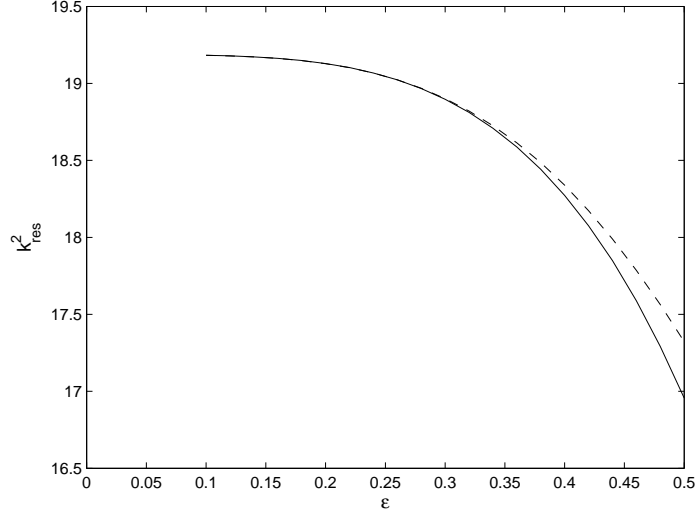


Figure 4: Asymptotic description $k_{res,a}^2(\varepsilon)$ (solid curve) and numerical description $k_{res,n}^2(\varepsilon)$ (dashed curve) for resonant energy $k_{res}^2(\varepsilon)$.

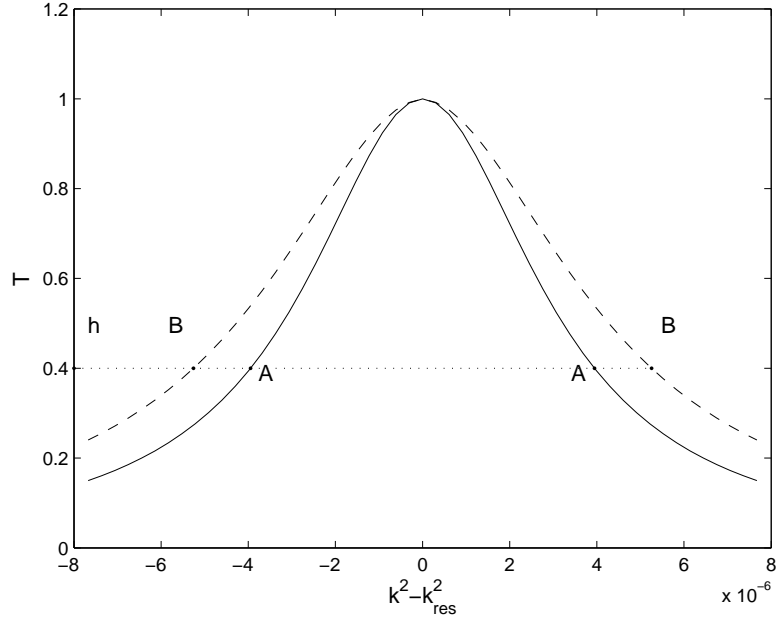


Figure 5: Transition coefficient for $\varepsilon = 0.2$: asymptotic description $T_a(k^2 - k_{res,a}^2)$ (solid curve) and numerical description $T_n(k^2 - k_{res,n}^2)$ (dashed curve) for transition coefficient $T(k^2 - k_{res}^2)$. The width of resonant peak at height h : asymptotic $\Delta_a(h, \varepsilon) = AA$; numerical $\Delta_n(h, \varepsilon) = BB$.

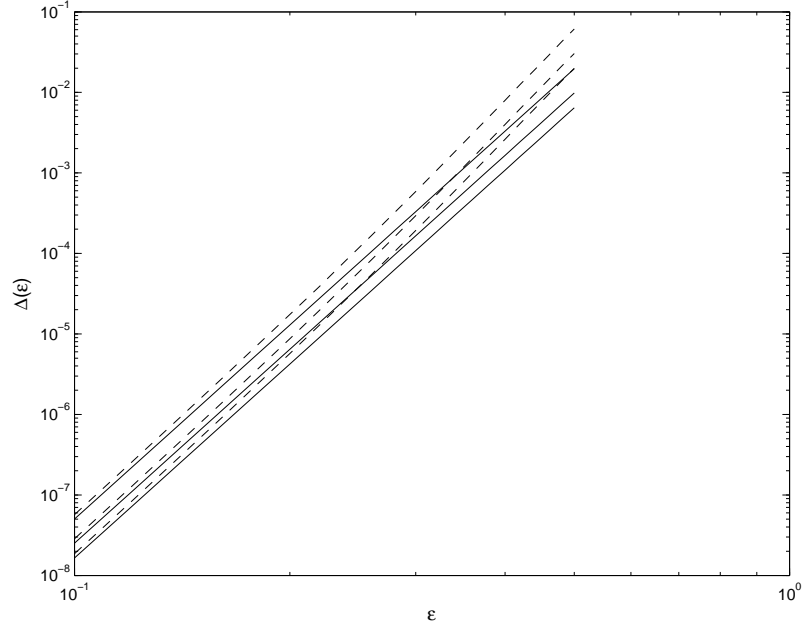


Figure 6: The width $\Delta(h, \varepsilon)$ of resonant peak for various h (dashed line for numerical description, solid line for asymptotic description): line 1 for $h = 0.2$; line 2 for $h = 0.5$; line 3 for $h = 0.7$.

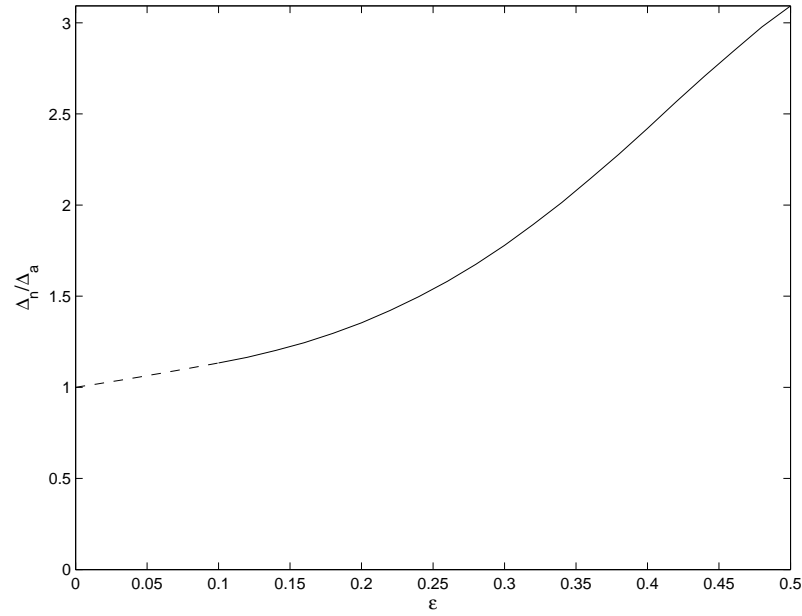


Figure 7: Ratio $\Delta_n(h, \varepsilon)/\Delta_a(h, \varepsilon)$ as function in ε . The ratio is independent of h within the accuracy of the analysis.

shows, for $\varepsilon \geq 0.5$ the resonant peak turns out to be so wide that the resonant tunneling phenomenon dies out by itself.

The forms of "asymptotic" and "numerical" resonant peaks are almost the same (see Fig. 5). The difference between the peaks is quantitatively depicted in Fig. 6. Moreover, it turns out that the ratio of the width $\Delta_n(h, \varepsilon)$ of numerical peak at height h to $\Delta_a(h, \varepsilon)$ of asymptotic peak is independent of h . The ratio as function in ε is displayed in Fig. 7.

Note that for $\varepsilon = 0.1$, i.e., at the left end of the band where the numerical and asymptotic results can be compared, the disparity of the results is more significant for the width of resonant peak than that for the resonant energy.

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